APPENDIX D: ROUND 3 DATA COMPARED TO THE ROUND 2 REPORT MECHANISTIC MODEL

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ROUND 3 DATA COMPARED TO THE ROUND 2 REPORT MECHANISTIC MODEL

As requested in US Environmental Protection Agency (EPA) comments on the Round 2 Report mechanistic model (EPA 2008), empirical tissue concentrations from the Round 3 dataset were compared to the predicted tissue concentrations from the calibrated mechanistic model developed as part of the Round 2 Report (Integral et al. 2007). The Round 3 tissue data were collected to fill gaps in spatial coverage of the Rounds 1 and 2 datasets and were not meant to be representative of Study Area-wide conditions. As such, they are not, strictly speaking, an appropriate "validation data set," but nonetheless it is useful to see how well the Round 2 model predicts the Round 3 data.

Table 1 compares the Round 3 dataset with the dataset used to calibrate the Round 2 Report mechanistic model (Rounds 1 and 2 tissue data). A comparison of Round 2 Report and updated model parameter values for key model parameters can be found in Appendix D (Section 7.0).

Table 1. Tissue Dataset Summary

	Number of Samples						
Dataset	**Clams (BIF)**	**Crayfish (EIC)**	**Sculpin**	**Largescale Sucker**	**Carp**	**Smallmouth Bass**	**Northern Pikeminnow**
Round 2 Report[a]	36	27	26	6	6	14	6
Round 3	7	5	12	0	9	18	0

[a] The dataset used for the Round 2 Report consisted predominantly of only Round 1 data. The only Round 2 data that were available were clam tissue data.

BIF – benthic invertebrate filter feeder

EIC – epibenthic invertebrate consumer

As shown in Table 1, no largescale sucker or northern pikeminnow were collected during Round 3 tissue sampling, so model performance could not be evaluated for these two species. Additionally, relatively few clam, crayfish, and sculpin samples were collected during Round 3 and these datasets are not representative of the Study Area-wide conditions to which the model was calibrated. The Round 3 sampling design was meant to fill data gaps and improve spatial coverage of the dataset on a whole, but the Round 3 dataset alone does not provide a good spatial coverage of the entire Study Area.

Table 2 presents species predictive accuracy factors (SPAFs, see Section 5.3.4 of the main report for a full description of this metric) for comparison of the model-predicted concentrations with both the Round 2 Report dataset (data from Round 1 and 2 tissue sampling) and the Round 3 dataset. This comparison is based on Study Area-wide SPAFs, which is why there is a single SPAF, even for receptors with small individual exposure areas.

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Table 2. Comparison of SPAFs from Round 2 Report and Using the Round 3 Data

Dataset	SPAF						
	Clams (BIF)	Crayfish (EIC)	Sculpin	Largescale Sucker	Carp	Smallmouth Bass	Northern Pikeminnow
Total PCBs							
Round 2 Report	5.6	**2.8**	**1.1**	1.3	2.0	**2.8**	**1.9**
Round 3 data	4.5	2.6	1.4	ND	3.6	**3.4**	ND
Total DDx							
Round 2 Report	3.4	**2.2**	1.1	1.1	**1.4**	4.5	**1.5**
Round 3 data	1.5	**12.5**	**5.5**	ND	**1.5**	**4.8**	ND
4,4′-DDD							
Round 2 Report	4.7	**2.6**	1.2	1.6	1.1	**2.3**	**1.5**
Round 3 data	1.8	**19.6**	**3.1**	ND	1.4	**1.9**	ND
Sum DDD							
Round 2 Report	5.0	**2.5**	1.4	1.8	1.4	**1.9**	**1.2**
Round 3 data	2.0	**17.0**	**2.8**	ND	1.6	**1.4**	ND
4,4′-DDE							
Round 2 Report	5.8	**1.3**	1.1	2.2	2.1	**2.1**	1.9
Round 3 data	3.6	**3.7**	**2.4**	ND	1.9	**2.7**	ND
Sum DDE							
Round 2 Report	4.9	**1.3**	1.1	1.9	1.8	**2.2**	1.8
Round 3 data	3.0	**4.1**	**2.6**	ND	1.6	**2.9**	ND
4,4′-DDT							
Round 2 Report	1.1	**13.5**	3.1	6.7	**1.5**	1.2	**1.8**
Round 3 data	**4.3**	**1109**	**6.8**	ND	**8.0**	1.3	ND
Sum DDT							
Round 2 Report	1.1	**5.4**	1.7	2.5	**3.0**	4.3	2.7
Round 3 data	**3.9**	**772**	**13.0**	ND	**11.2**	**3.6**	ND

[a]   **SPAFs** shown in **bold** indicate that the model was over-predicting for this species-chemical combination.
BIF – benthic invertebrate filter feeder
DDD – dichlorodiphenyldichloroethane
DDE – dichlorodiphenyldichloroethylene
DDT – dichlorodiphenyltrichloroethane
EIC – epibenthic invertebrate consumer
ND – no data
SPAF – species predictive accuracy factor
total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

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Overall, SPAFs from the Round 2 Report and SPAFs calculated using the Round 3 data were generally similar, indicating that model calibration is appropriate. However, there were several cases when the SPAFs for the Round 3 dataset were significantly higher than the SPAFs for the dataset from the Round 2 Report:

- Crayfish SPAFs for 4,4′-DDD, Sum DDD, 4,4′-DDT, Sum DDT, and total DDx

- Sculpin SPAFs for 4,4′-DDT and Sum DDT

- Carp SPAFs for 4,4′-DDT and Sum DDT

There were two main reasons for these high SPAFs. First, the Round 3 dataset is not representative of Study Area-wide conditions for the small-home-range species (n = 5 for crayfish and n = 12 for sculpin, as compared to n = 27 and n = 26, respectively, in the Round 2 Report dataset). And second, improved analytical methods used during the Round 2 and 3 datasets greatly increased detection frequencies and consequently lowered the Study Area-wide average concentrations of the empirical data, indicating the need to recalibrate the model to incorporate the new information obtained by achieving lower detection limits in Round 3.[1] Table 3 shows the detection frequencies and the Study Area-wide average concentrations for the species-chemical pairs listed above.

Table 3. Detection Frequencies and Average Concentrations

	Detection Frequency (Average Concentration [µg/kg dw])					
	Crayfish (EIC)		Sculpin		Carp	
Chemical	**Round 2 Report**	**Round 3 Dataset**	**Round 2 Report**	**Round 3 Dataset**	**Round 2 Report**	**Round 3 Dataset**
4,4′-DDD	19% (1.7)	100% (0.22)	NA	NA	NA	NA
Sum DDD	19% (1.9)	100% (0.28)	NA	NA	NA	NA
4,4′-DDT	30% (2.2)	20% (0.027)	81% (102)	100% (4.9)	17% (6.6)	100% (1.2)
Sum DDT	74% (4.6)	20% (0.032)	85% (127)	100% (5.8)	17% (10.7)	100% (2.8)
Total DDx	100%[a] (14.1)	100% (2.5)	100%[a] (222)	100% (35.2)	NA	NA

[a]   Although the detection frequency for total DDx is 100% for the Round 2 Report dataset, this indicates only that one of the six components of this total was detected. The detection frequency for 4,4'-DDE was high in the Round 2 Report dataset because it is generally present at higher concentrations.

DDD – dichlorodiphenyldichloroethane
DDT – dichlorodiphenyltrichloroethane
EIC – epibenthic invertebrate consumer

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[1] Round 1 tissue samples were analyzed for pesticides using the SW8081/8270 method. With the exception of whole-body juvenile Chinook salmon, which were also analyzed using the SW8081/8270 method, all Round 2 (clam only) and Round 3 tissue samples were analyzed for pesticides by Axys using a high resolution analytical method (MLA-028) to reduce reporting limits.

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NA – not applicable

total DDx – sum of all six DDT isomers (2,4′-DDD, 2,4′-DDE, 2,4′-DDT, 4,4′-DDD, 4,4′-DDE and 4,4′-DDT)

As can be seen from Table 3, the Round 3 average tissue concentrations for total DDxs for several species are significantly lower than those used in the Round 2 Report as a result of the improved detection frequencies (and thus lower detected concentrations). The results of this evaluation indicate that the Round 2 Report mechanistic model is able to reasonably predict Round 3 tissue concentrations, except in cases where the Round 3 data were not spatially representative and/or there were significant analytical differences between the two datasets.

REFERENCE

EPA. 2008. EPA letter and attachment dated August 8, 2008 to Lower Willamette Group (from E. Blischke and C. Humphrey to J. McKenna and R. Wyatt) regarding Portland Harbor RI/FS: comments on Appendix E - Comprehensive Round 2 Site Characterization and Data Gaps Analysis Report. US Environmental Protection Agency Region 10, Oregon Operations Office, Portland, OR.

Integral, Windward, Kennedy/Jenks, Anchor. 2007. Portland Harbor RI/FS: Comprehensive round 2 site characterization summary and data gaps analysis report, plus addenda. IC07-0004. Prepared for Lower Willamette Group. Integral Consulting, Inc., Mercer Island, WA; Windward Environmental LLC, Seattle, WA; Kennedy/Jenks Consultants, Portland, OR; Anchor Environmental, LLC, Portland, OR.

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